Neocedranol

Inchi: InChI=1S/C15H26O/c1-9-5-6-13-14(3,4)11-7-15(9,13)8-12(16)10(11)2/h9-13,16H,5-8H2,
InchiKey: AEJKOZRRMKOBQS-UYNSMTERSA-N
Formula: C15H26O
SMILES: CC1C(O)CC23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	54.83	kJ/mol	Joback Method
hf	-349.96	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.466		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	645.34	K	Joback Method
tc	851.43	K	Joback Method
tf	397.25	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.58	J/mol×K	645.34	Joback Method
cpg	621.09	J/mol×K	679.69	Joback Method
cpg	640.66	J/mol×K	714.04	Joback Method
cpg	659.50	J/mol×K	748.38	Joback Method
cpg	677.83	J/mol×K	782.73	Joback Method
cpg	695.86	J/mol×K	817.08	Joback Method
cpg	713.82	J/mol×K	851.43	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202816&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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